THEORETICAL INVESTIGATION OF THE X-RAY STARK EFFECT IN SMALL MOLECULES

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We perform a computational study of the Stark effect for X-ray absorption spectra, and analyze the electric field response through the orbital and geometry variation with the electric field strength and orientation. We utilize a combination of Q-Chem and CFOUR, using the powerful CVS-EOM-CCSD/aug-cc-pCVTZ method for treating the vertical x-ray absorption energies and transition properties. External electric fields are applied collinear to the molecular dipole moment and the molecular geometry and orientation (when allowed by symmetry) are optimized in the presence of the field. We discuss how the symmetry of the molecule affects the X-ray spectra and identify characteristic features for the finite-field spectra. A rich structure is observed in the variation of X-ray spectra with varying electric field strength.